

Final Inventory Report
(NAG-1-02076)

on

Characterization on Smart Optics using Ellipsometry

for

Project Period: April 1, 2002 – July 31, 2002

Submitted by:
Principal Investigator, Dr. Kyo D. Song

Department of Technology
Center for Materials Research
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Introduction

Recently, NASA Langley Research Center developed a smart active optical concept to filter narrow band pass or to control optical intensity. To characterize developed smart optics materials, we have measured thickness and reflection properties of the materials using a WVASE32 ellipsometry. This project allowed us to:

- Prepare the smart optical materials for measurement of thickness and optical properties at NASA Langley Research Center
- Measure thickness and optical properties of the smart optical materials.
- Evaluate the measured properties in terms of applications for narrow band-pass filters

The outcomes of this research provide optical properties and physical properties of the smart optics on a selected spectral range. The applications of this development were used for field-controlled spectral smart filters.

Principle of Ellipsometry

Ellipsometry is an optical technique for determining properties of surfaces and thin films. This experiment measures intensities of reflected or transmitted light or polarization states. These quantities may affect by the physical parameters such as thickness or optical constants. For example, Ellipsometry measures the ratio of Fresnel reflection coefficients R_p and R_s for p- and s- polarized light, respectively. Let's define the complex ellipsometric parameter ρ .

$$\rho = \frac{R_p}{R_s} \quad 1)$$

The ellipsometric parameter ρ is only a function of the Fresnel reflection coefficients of the sample. ρ is commonly expressed in terms of the two real-valued ellipsometric parameters ψ and Δ as follows:

$$\rho \equiv \tan \psi \exp(i\Delta) \quad 2)$$

such that $\tan \psi$ equals the magnitude of the ratio of the p- to s-direction complex reflection coefficients for the sample, and Δ is the phase difference between the p- and s-reflection coefficients.

To measure thickness of sample in a single film, a solution of the electric field wave equation from Maxwell's equation in the E & M plane wave can be written as,

$$E(r,t) = E_0 \exp\left(\frac{i2\pi n}{\lambda} q \cdot r\right) \exp(-i\omega t) \quad 3)$$

where q is a unit vector along the direction of wave propagation, n is the complex index of refraction, λ is the wavelength of the light in vacuum, ω is the angular frequency of the wave, and E_0 is a complex vector constant specifying the amplitude and polarization state of the wave.

It is a simple matter to show that propagation of a wave across the film yields a resulting wave of the following form.

$$E_{after} = E_{before} \cdot \exp(-i2\beta), \quad 4)$$

where, β is the phase thickness (or optical thickness) of the film for the given wavelength and angle of incidence), given by

$$\beta = 2\pi n_1 \frac{d}{\lambda} \cos \phi_1 = 2\pi \frac{d}{\lambda} \sqrt{n_1^2 - n_0^2 \sin^2 \phi_0} \quad 5)$$

in which d is the film thickness and λ is the wavelength, in same units as the film thickness. Similarly, the successive reflected light can be calculated and summing the reflected lights. Therefore, the expected Ψ and Δ in equation 2) for a single film sample at a given wavelength and angle of incidence may be calculated as follows;

1. calculate β from equation 5)
2. calculate the p-plane reflection coefficients for ambient and the film from Snell's law
3. Evaluate Ψ and Δ in equation 2)

Ellipsometry is a model dependent technique in that the measured quantities are the physical quantities to determine, and numerical analysis of the experimental data on some mathematical model is required to obtain useful physical information about the sample. For this process, WVASE32 uses the mean-squared method to minimize errors.

Using Ellipsometry, the following parameters can be determined as,

- Optical constants (n and k)
- Thin film thickness
- Doping concentration
- Surface and Interfacial roughness
- Growth rate (in-situ)
- Temperature (in-situ)

The regimes of applicability

The choice of ellipsometry is determined by the best wavelength range to meet given application. It works best for film characterization when the film thickness is not too smaller or larger than the wavelength of the light used. For example, it is relatively difficult to characterize a 0.5 nm with a 500 nm wavelength of the probe light. In general, an infrared ellipsometry is best for thickness about 100 nm – 50 μ m, while visible and UV lights are best for 10 nm – 1 μ m.

Procedure of Measurement

All ellipsometry have a light source and end with a detector. There are, in general, a polarizer, a retarder, and a compensator between the light source and the detector. If linearly polarized light of a known orientation is reflected at oblique incidence from a surface the reflected (or transmitted) light is elliptically polarized. The shape and orientation of the ellipse depend on the angle of incidence, the direction of the polarization of the incident light, and the reflection properties of the surface. The variation of polarization of the reflected light with a quarter-wave plate followed by an analyzer, the orientations of the quarter-wave plate (retarder) can be measured until no light passes through the analyzer. WVASE32 is a rotating analyzer ellipsometry that could allow the measurement of the polarization state of the reflected light.

Application of smart optics

The smart optics is a dynamic filter and its concept is based on the constraint of quantum electronic behavior (weakly) and dipole moment change (strongly) in a thin-film or quantum-dot domain of materials that are effectively controlled by externally applied fields such as electric field or magnetic field.

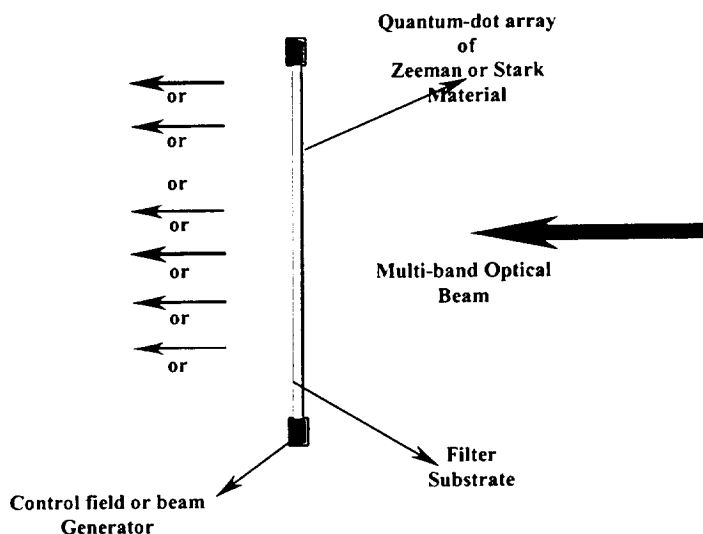


Fig. 1 Concept of Smart Optics (after Choi)

Quantum Electronic Constraint – Electric Field Effects:

The effects on atomic and molecular energy level and spectra by externally imposed field give rise to radiative transitions as a consequence of higher order perturbation. Hence, the effect by higher order perturbation results in a weak interaction mainly to atomic level. This effect is generally called as the Stark effect [1]. When an electric field is used, it appears like

the electrochromic effect but fundamentally different from the fact that electrochromism is based on the ionic state changes that give rise to the colored or bleached state from either anodic or cathodic charge. The constraint to quantum electronic behavior of atoms and molecules under an applied field is represented by the Stark effect as stated above and can be effectively used for selective spectral transmission in a filtering mechanism by state control through an externally applied field.

Quantum Electronic Constraint – Magnetic Field Effects: The effect on dipole moment of atoms or molecules by an externally applied magnetic field is often called as the Zeeman effect [2] and appears as level multiplicities and nuclear spins. Because of dipole interaction, the angular momentum vector (L) processes around the field vector as a coupling with spin-orbit momentum vector (S) when Zeeman energy is much less than spin-orbit interaction energy. However, as the field effect increases (or the Zeeman energy increases), the angular and spin-orbit momenta individually are decoupled, thus resulting in destroying the spherical symmetry of the total Hamiltonian and producing a splitting linear with the field strength. In such a case, the magnetic (M) or Zeeman momentum strongly dictates degeneracy and controls level multiplicities (or level splittings) and nuclear spins, resulting in spectral variations. The optical transitions by the Zeeman effect encompass emission, absorption, and transmission spectra within atomic or molecular structures. Hence, the impinging quanta of spectra on or through Zeeman materials can be selectively gated for the color options rather than bleach (flux density control) by modulating externally applied fields.

Effects of Quantum-Dot Domain: In quantum-dots [3] that contain a small and controllable number (1~1000) of electrons, the electronic states are completely quantized due largely to the quantum confinement, the resonant structure associated with confinement, and granular nature of electric charge. The density of (quantum) states is uniquely populated on discrete energy levels (Dirac δ -function) in quantum-dots unlike quantum-wells or quantum-lines. Therefore, the behavior of electrons in quantum-dots can be controlled by either electric or magnetic field, but only within discrete levels of energy spectrum that allows optical transitions even without Zeeman effect (spin

splitting). There are many reported works [4] that proved optical transitions of II-VI and III-V materials with or without the applied field.

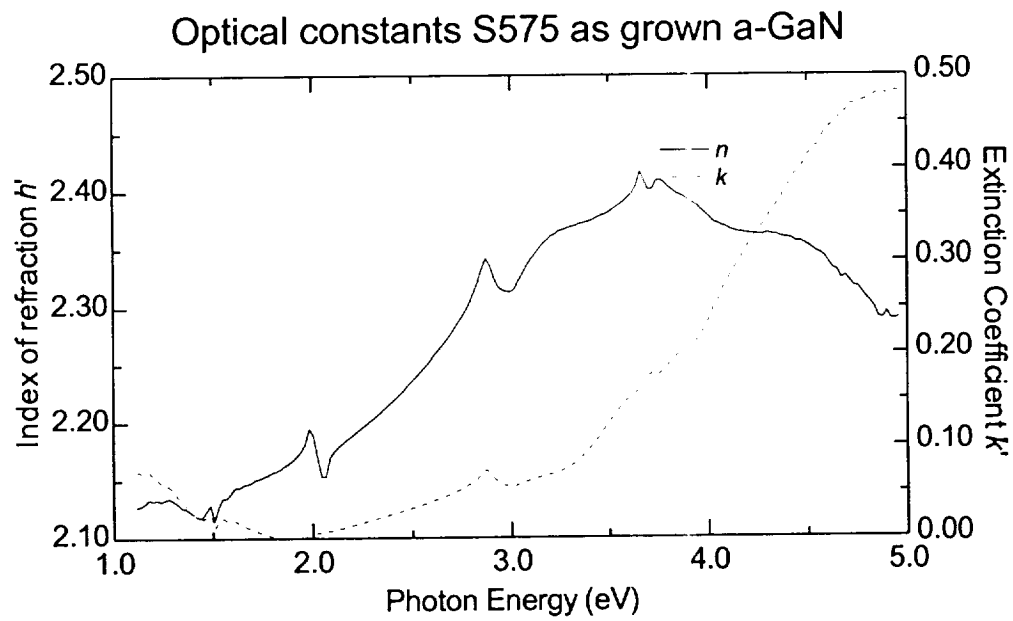
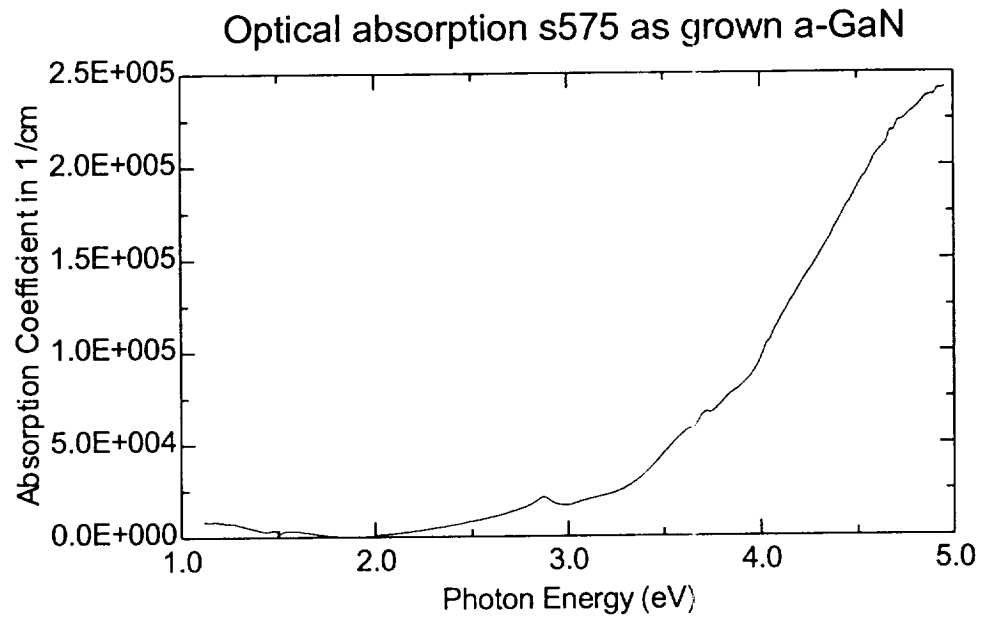
Organic Materials with Quantum Effects: The organic crystals, similarly with II-VI and III-V materials show very interesting optical and electronic properties that are dictated by excitons. An exciton is a bound electron-and-hole pair that transports energy through a solid. Three different forms of exciton exist, such as Frenkel, Wannier-Mott, and charge-transfer varieties. The Frenkel exciton is a molecule in an excited state and commonly observed in molecular organic materials. The Wannier-Mott exciton is a hydrogenic state where the electron is delocalized from the hole and normally found in semiconductors. The charge transfer exciton is the co-pair state of electron-hole that resides on adjacent molecules. The bound excitonic state of ordered organic crystalline structure (i.e. aluminum tris[8-hydroxyquinoline] or Alq₃) exhibit electroluminescence (EL) and photoluminescence (PL) under the injection of electron-hole pair injection [5].

Figure 1 shows the description of the concept of smart optics. The array formation of Zeeman or Stark material quantum-dots or thin-film organic crystal could be developed on an optical window substrate for smart active optical filtering. The thickness of quantum-dots is of tens of nanometers.

Materials Growth in the Lab

GaN and related group III-nitride compounds became recently intensively studied III-V semiconductors, due to the broad spectrum of optical and electronic applications. Commercially available devices (e.g. blue light emitting diodes) are prepared on the base of hetero-epitaxial III-nitride compound structures grown on sapphire and SiC substrates. As the result of large lattice mismatch, these structures contain a very high density of various defects (e.g. dislocations, nanopipes, inversion domains). Homo-epitaxial GaN films are still scarce, because of the lack of commercially available high quality single GaN crystals. This has been a limiting factor for detailed and reliable studies of the physical properties of this material. However, Dr. Little, a Research Associate at NASA LaRC, developed a CVD system to growth GaN single crystals for smart optics. The proposed research is to analyze materials grow from the system and provide optical properties of the materials. During the grant period, a GaN on Si substrate is analyzed with an ellipsometry in the laboratory as shown in figs. 2 and 3.

Typical Measurement of GaN on Si (Fig. 2: Absorption, Fig.3.:Index of refraction)



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